Performance enhancements in MFDn

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U.S. DEPARTMENT OF ENERGY
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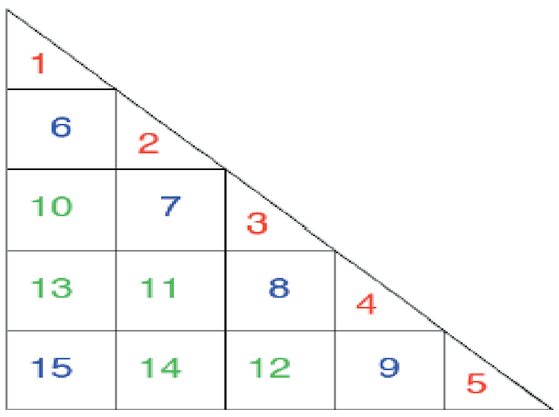
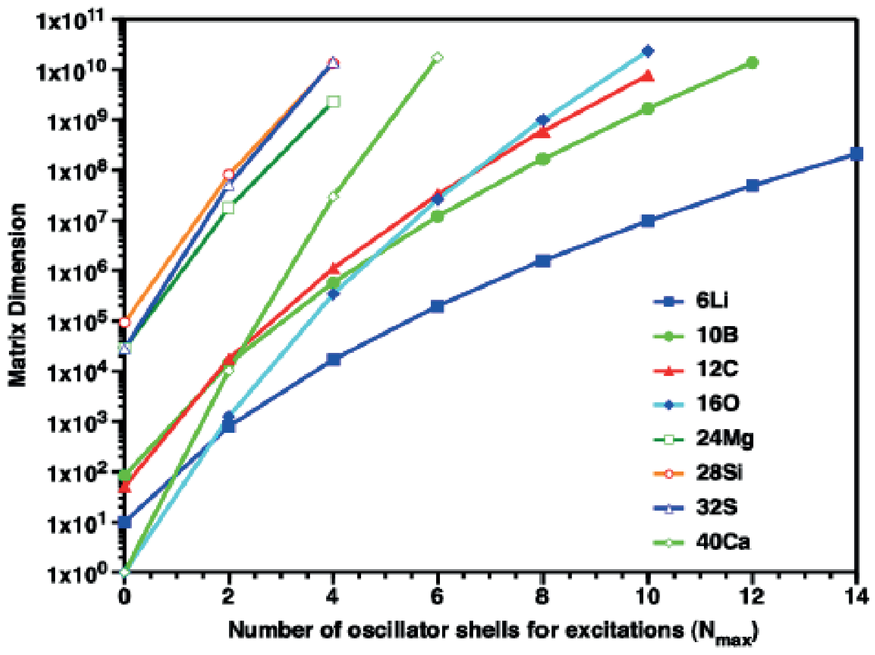
MFDn overview

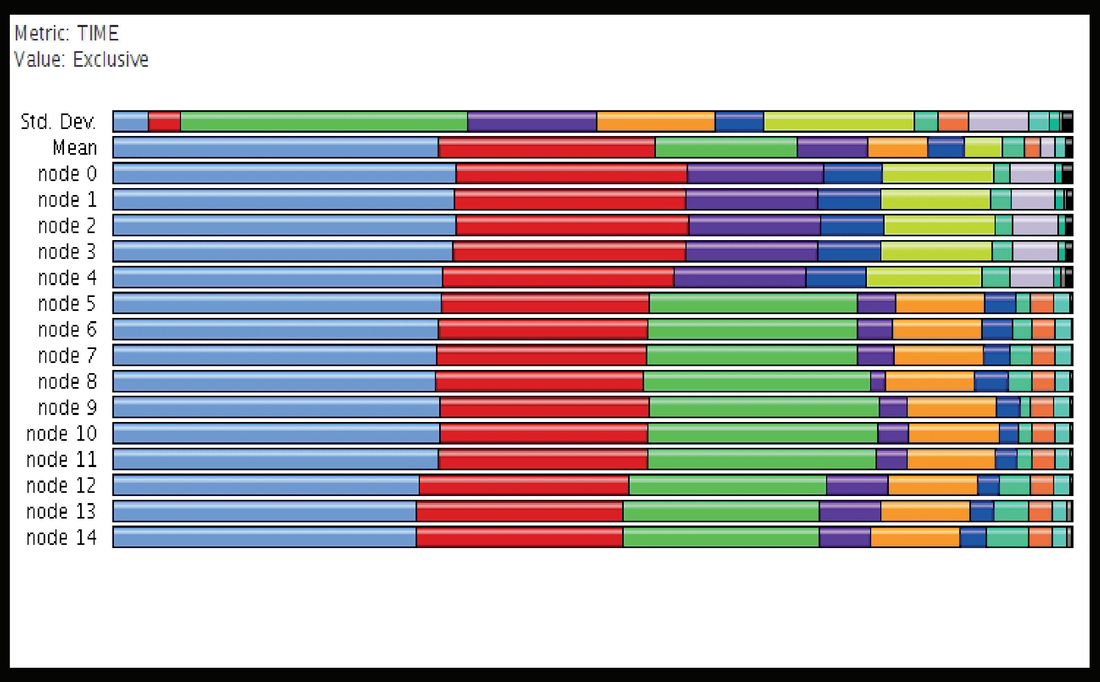
- MFDn – Many Fermion Dynamics for nuclear structure – developed at Iowa State University.
- State of the art parallel code for ab-initio nuclear structure calculations.
- Evaluates the nuclear Hamiltonian in a large harmonic oscillator basis.
- The low-lying spectra of large sparse Hamiltonian matrix is obtained by the Lanczos diagonalization procedure to obtain lowest energy levels and corresponding wave functions.
- Some of the largest problem sizes which MFDn has been used to solve are summarized below.
  - ^{14}Be; N_{max} = 8; matrix dimension 2,790,412,009.
  - ^{14}F; N_{max} = 8; matrix dimension 1,990,061,078.
  - ^{14}N; N_{max} = 8; matrix dimension 1,090,393,922.

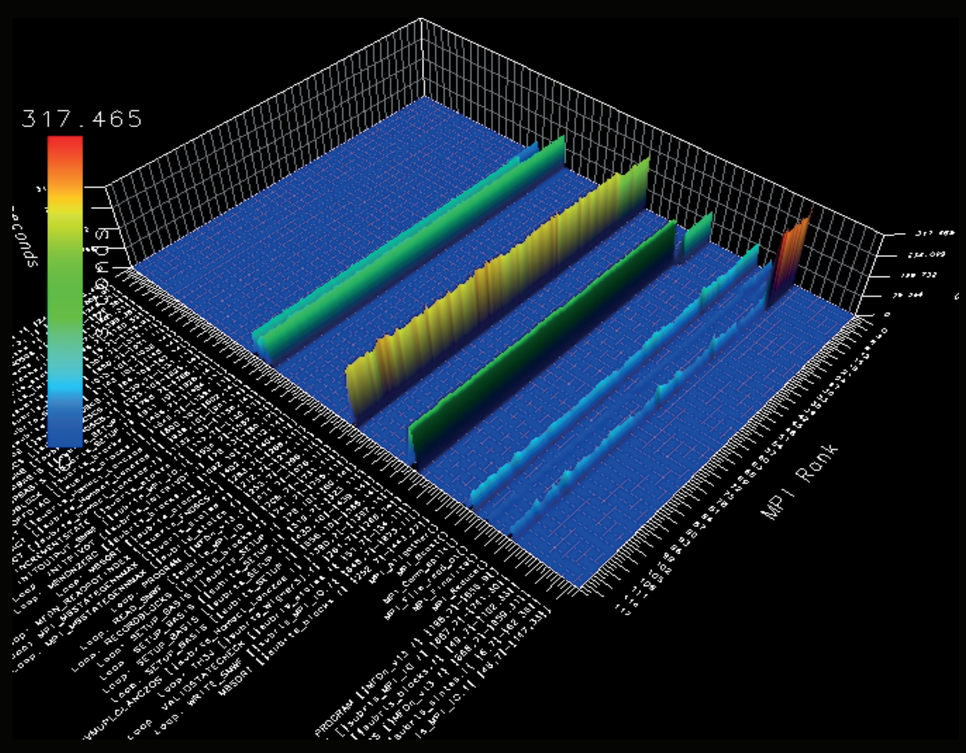


- 2D matrix distribution over all processors, only lower triangle stored and used (since matrix is symmetric).
- Runs on *n(n+1)/2* processors, where *n* is the number of diagonal processors (shown in red in Fig)



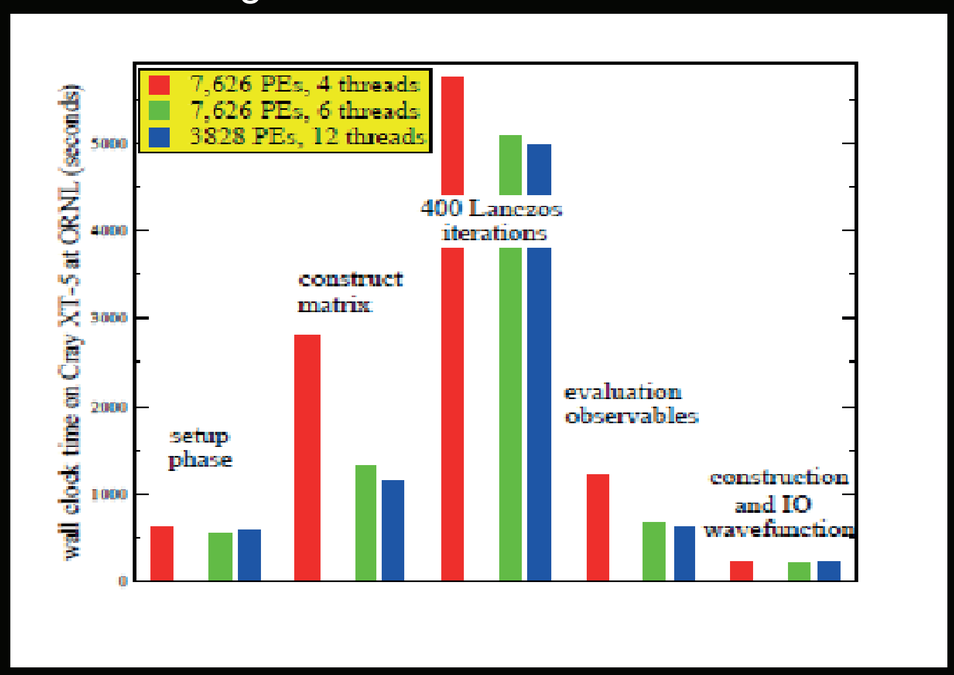
Performance data gathered by TAU on Franklin (NERSC) for ^{12}C N_{max} = 4 running on 15 MPI processors

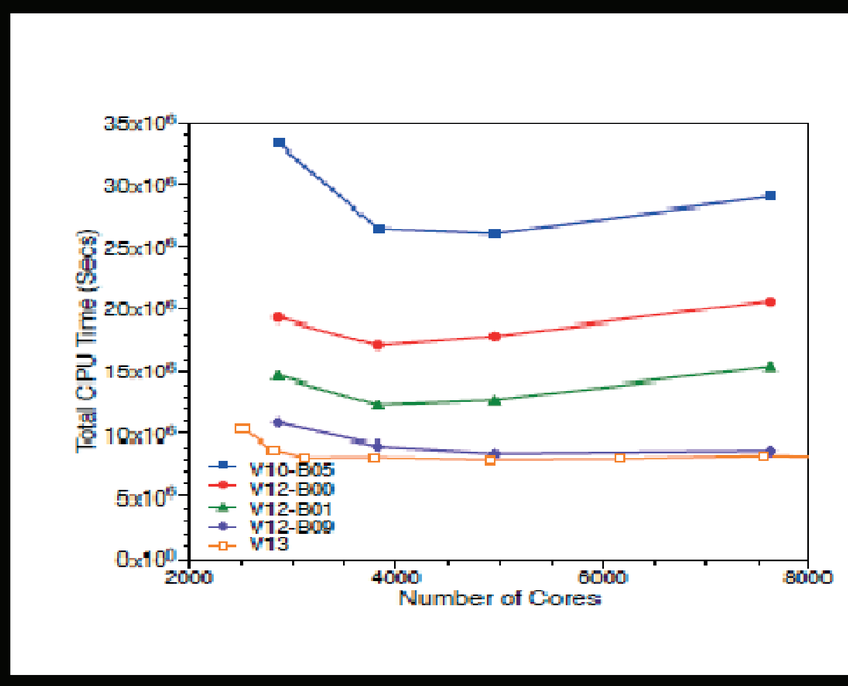




Parallel Performance

- Recent algorithmic and code optimization developments – increase in MFDn parallel performance.
  - during last 4 years under the U.S. Department of Energy SciDAC-2 Program.





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